



A Note on Some Growth Curves Arising from Box–Cox Transformation

Nikolay Kyurkchiev and Anton Iliev

Abstract— Mathematical models of growth have been developed a long period of time. Estimating the lag time in the growth process is a practically important problem. In this note we provide estimates for the one-sided Hausdorff approximation ($t_{new-lag}$) of the shifted step-function by sigmoidal function arising from Box–Cox transformation. We present a software module (intellectual property) within the programming environment of *CAS Mathematica* for analysis of growth curves. Numerical examples, illustrating our results are given, too.

Keywords— Sigmoidal function, Step function, Hausdorff distance, Box–Cox transformation, Lag time

I. INTRODUCTION

Growth curves are found in a wide range of disciplines, such as biology, chemistry, ecology, forestry, agriculture, medical science and many other fields for describing the growth of organisms and populations [4].

Garcia [1], [2] presented a generalized model, depending on two shape parameters, that includes most of the common growth functions as special cases.

Let B is the transformation [3]

$$B(x, c) = \begin{cases} \frac{1-x^c}{c}, & \text{if } c \neq 0, \\ -\ln x, & \text{if } c = 0. \end{cases} \quad (1)$$

The inverse transformation is

$$B^{-1}(x, c) = \begin{cases} (1-cx)^{\frac{1}{c}}, & \text{if } c \neq 0, \\ e^{-x}, & \text{if } c = 0 \end{cases} \quad (2)$$

defined for $cx \leq 1$.

Consider

$$B(B(y, a), b) = t \quad (3)$$

Solving for y gives the yield equation

$$y = B^{-1}(B^{-1}(t, b), a) \quad (4)$$

or

$$y = \lim_{t_1 \rightarrow a, t_2 \rightarrow b} \left(1 - t_1 (1 - t_2 t)^{\frac{1}{a}} \right)^{\frac{1}{b}}.$$

More explicitly [1],

$$y = \begin{cases} \left(1 - a(1-bt)^{\frac{1}{b}} \right)^{\frac{1}{a}} & \text{if } a, b \neq 0 \end{cases} \quad (5)$$

$$y = e^{-(1-bt)^{\frac{1}{b}}} \text{ if } a = 0, b \neq 0 \quad (6)$$

$$y = (1 - ae^{-t})^{\frac{1}{a}} \text{ if } a \neq 0, b = 0 \quad (7)$$

$$y = e^{-e^{-t}} \text{ if } a, b = 0. \quad (8)$$

The models (5)–(8) includes some models such as Logistic, Monomolecular, Bertalanfy, Exponential, Gompertz, Richards, Chapmann–Richards, Schnute, Stannard and their modifications.

The growth models are described by free parameters a and b , each contributing to the characteristics of the sigmoidal function.

The function (5) finds applications in many scientific fields, including population dynamics, bacterial growth, population ecology, plant biology and statistics.

Further for $a \neq 0$ we have

$$y'(t) = y^{1-a} \left(\frac{1-y^a}{a} \right)^{1-b},$$

$$y''(t) = \frac{1}{a^{1-b}} (1-y^a)^{-b} \left((1-a)y^{-a}(1-y^a) - a(1-b) \right)$$

and the y - position of the inflection point, if it exists, is

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$$y_{infl} = \left(\frac{1-a}{1-ab} \right)^{\frac{1}{a}}.$$

The curve (5) is a sigmoid for $a < 1, b \leq 0$ and $ab < 1$.

Estimating the lag time in the growth process is a practically important problem [5], [6].

The lag time - t_{lag} (see Fig. 1) is estimated by extending the tangent at inflection point to the initial baseline.

The curve is typically divided into the lag phase, the growth phase, and the plateau phase.

We study the sigmoid function

$$L(t; a, b, \gamma) = \begin{cases} \left(1 - a(1 - b(t - \gamma))^{\frac{1}{b}} \right)^{\frac{1}{a}} & \text{if } a, b \neq 0 \end{cases} \quad (9)$$

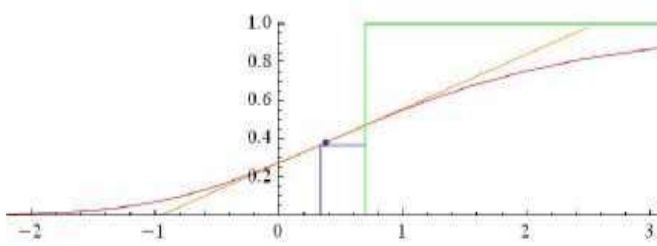


Figure 1: Definitions: a) t_{lag} - is estimated by extending the tangent at inflection point to the initial baseline; b) $t_{new-lag}$ - the one-sided Hausdorff approximation - d of the shifted step-function by sigmoidal function (9). The parameters are: $a = -0.7, b = -0.2, \gamma = 0.7; d = 0.365457$.

In this note we prove estimates for the one-sided Hausdorff approximation ($t_{new-lag}$) of the shifted step-function by sigmoidal function (9).

Let us point out that Hausdorff distance is the most natural measuring criteria for the approximation of bounded discontinuous function [7], [8].

Definition 1. Define the shifted step function h_γ as:

$$h_\gamma(t) = \begin{cases} 0, & \text{if } t < \gamma, \\ [0, 1], & \text{if } t = \gamma, \\ 1, & \text{if } t > \gamma. \end{cases} \quad (10)$$

Definition 2. The Hausdorff distance (H-distance) $\rho(f, g)$ between two interval functions f, g on $\Omega \subseteq \mathbb{R}$, is the distance between their completed graphs $F(f)$ and

$F(g)$ considered as closed subsets of $\Omega \times \mathbb{R}$ [9], [10]. More precisely,

$$\rho(f, g) = \max \left\{ \sup_{A \in F(f)} \inf_{B \in F(g)} \|A - B\|, \sup_{B \in F(g)} \inf_{A \in F(f)} \|A - B\| \right\}, \quad (11)$$

wherein $\|\cdot\|$ is any norm in \mathbb{R}^2 , e. g. the maximum norm $\|(t, x)\| = \max\{|t|, |x|\}$; hence the distance between the points $A = (t_A, x_A)$, $B = (t_B, x_B)$ in \mathbb{R}^2 is $\|A - B\| = \max(|t_A - t_B|, |x_A - x_B|)$.

II. MAIN RESULTS

We study the one-sided Hausdorff approximation of the shifted step function $h_\gamma(t)$ by sigmoidal function $L(t; a, b, \gamma)$.

The following Theorem is valid

Theorem 2.1 For the one-sided Hausdorff distance d between the function $h_\gamma(t)$ and the function (9) the following hold:

$$d \approx d^* \quad (12)$$

where d^* is the unique positive solution of the equation

$$(1-a)^{\frac{1}{a}} - \left(1 + (1-a)^{\frac{1}{a-1}} \right) d - \frac{b(1-a)^{\frac{1}{a}}}{2(a-1)} d^2 = 0. \quad (13)$$

Proof. The one-sided Hausdorff distance d satisfies the relation (see, Figure 1)

$$L(\gamma - d) = \left(1 - a(1 + bd)^{\frac{1}{b}} \right)^{\frac{1}{a}} = d. \quad (14)$$

Let us examine the function

$$F(d) = \left(1 - a(1 + bd)^{\frac{1}{b}} \right)^{\frac{1}{a}} - d. \quad (15)$$

Consider function

$$G(d) = (1-a)^{\frac{1}{a}} - \left(1 + (1-a)^{\frac{1}{a-1}} \right) d - \frac{b(1-a)^{\frac{1}{a}}}{2(a-1)} d^2. \quad (16)$$

From Taylor expansion

$$\left(1 - a(1 + bd)^{\frac{1}{a}}\right)^{\frac{1}{a}} - d = (1 - a)^{\frac{1}{a}} - \left(1 + (1 - a)^{\frac{1}{a-1}}\right) d - \frac{b(1 - a)^{\frac{1}{a}}}{2(a - 1)} d^2 + O(d^3)$$

we obtain $G(d) - F(d) = O(d^3)$ (see, Fig. 2).

From Descartes' rule of signs the equation (13) has unique positive root.

This completes the proof of the theorem.

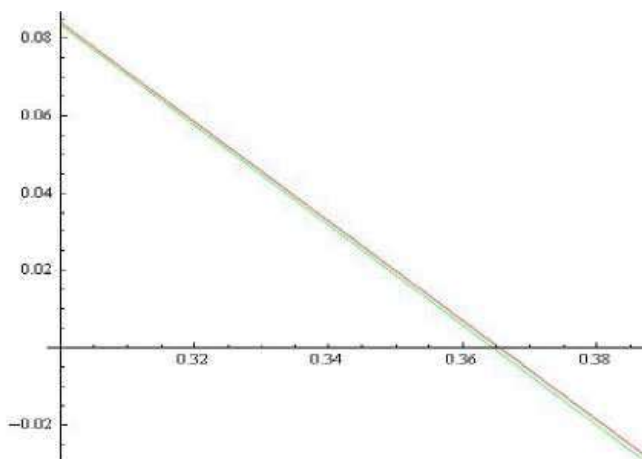


Figure 2: The functions $F(d)$ and $G(d)$ for $a = -0.7$, $b = -0.2$, $\gamma = 0.7$.

The bound for d computed by nonlinear equation (15) is $d = 0.365457$. From (12)–(13) we have $d \approx d^* = 0.364463$.

The "new" lag time is then given in terms of the one-sided Hausdorff distance - d .

III. CONCLUSION REMARKS

The Hausdorff approximation of the interval step function by the logistic and other sigmoid functions is discussed from various approximation, computational and modelling aspects in [11]–[21].

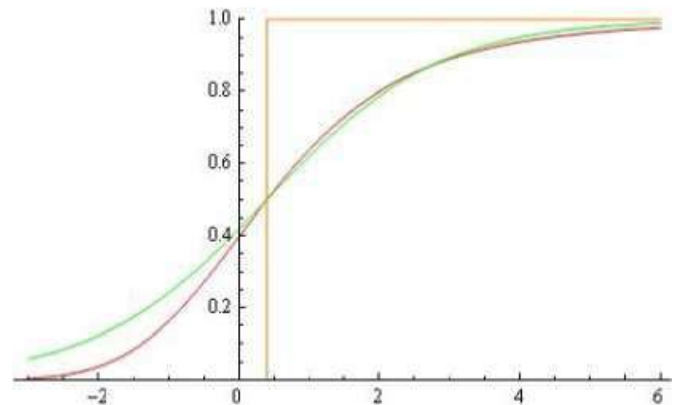


Figure 3: Comparison of the sigmoid function (9) (red) and Verhulst logistic function (green) for $\gamma = 0.4$, $b = -0.2$, $a = -1$ and $k = 0.82$.

Some comparison of the sigmoid curve (9) (for $a = -1$)

$$L(t; -1, b) = \frac{1}{1 + (1 - b(t - \gamma))^{\frac{1}{b}}}$$

and Verhulst logistic function

$$V(t; k) = \frac{1}{1 + e^{-k(t - \gamma)}} \text{ is plotted in Fig. 3.}$$

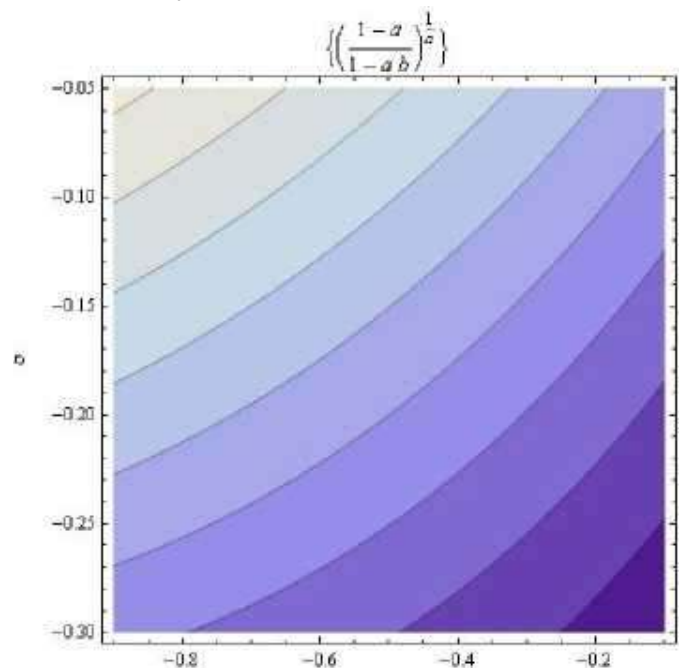


Figure 4: The ContourPlot for the y -position of the inflection point.

The *ContourPlot* (in *CAS Mathematica*) for y – position of the inflection point is displayed in Fig. 4.

```

γ = Input[" γ ":{0.7}];
Print[" γ = ", γ];
a = Input[" a ":{-0.7}];
Print[" a = ", a];
b = Input[" b ":{-0.2}];
Print[" b = ", b];
Print["The following nonlinear equation is used to determination of
the one-sided Hausdorff distance between shifted step function and
shifted growth curve - d (the new_lag_time): "];
Print[" (1-a*(1+b*d)^(1/b))^(1/a)-d=0 "];
FindRoot[(1-a*(1+b*d)^(1/b))^(1/a)-d, {d, 0}]

γ = 0.7
a = -0.7
b = -0.2
The following nonlinear equation is used to determination of
the one-sided Hausdorff distance between shifted step function and
shifted growth curve - d (the new_lag_time):
(1-a*(1+b*d)^(1/b))^(1/a)-d=0
{d -> 0.365457}

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Figure 5: Simple module implemented in *CAS Mathematica* for calculation of the value of the one–sided Hausdorff distance – d .

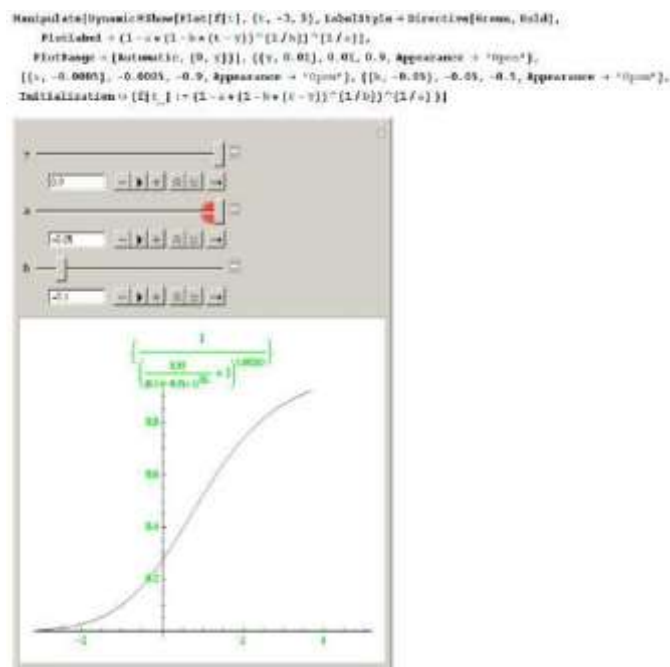


Figure 6: The software tool for animation and visualization in *CAS Mathematica*.

As an example of such a tool we propose a software module within the programming environment of *CAS Mathematica*.

The module offers the following possibilities: i) generation of the sigmoid curves arising from Box–Cox transformation; ii) when user-defined values for a, b, γ are given "check sigmoid curves"; iii) analysis of the y -component of the inflection point (contour plot) and the classic definition of $t_{lag-time}$; iv) numerical calculation of magnitude of one–sided Hausdorff distance in light of the "new researches" - $t_{new-lag-time}$; v) software tools for animation and visualization. The proposed module allows uniformity treatment of sigmoid curves generated by the transformation of the Box–Cox and hopefully, this will limit self-oriented researches of growth curves, which will appear in the literature.

REFERENCES

- [1] O. Garcia, Unifying sigmoid univariate growth equations, *Forest Biometry, Modelling and Information Sciences 1* (2005) 63–68
- [2] O. Garcia, Visualization of a general family of growth functions and probability distributions - The Growth–curve Explorer, *Environmental Modelling and Software 23* (2008) 1474–1475
- [3] G. Box, D. Cox, An analysis of transformations, *Journal of the Royal Statistical Society, B 26* (1964) 211–252
- [4] G. Seber, C. Wild, *Nonlinear Regression*, Wiley–Interscience, New York (2003)
- [5] S. Shoffner, S. Schnell, Estimation of the lag time in a subsequent monomer addition model for fibril elongation, *bioRxiv The preprint server for biology*, (2015) 1–8, doi:10.1101/034900
- [6] P. Arosio, T. P. J. Knowles, S. Linse, On the lag phase in amyloid fibril formation, *Physical Chemistry Chemical Physics 17* (2015) 7606–7618, doi:10.1039/C4CP05563B
- [7] R. Angelov, S. Markov, Hausdorff Continuous Interval Functions and Approximations, In: M. Nehmeier et al. (Eds), *Scientific Computing, Computer Arithmetic, and Validated Numerics*, 16th International Symposium, Springer, SCAN 2014, LNCS 9553 (2016) 3–13, doi:10.1007/978-3-319-31769-4
- [8] N. Kyurkchiev, A. Andreev, Approximation and antenna and filter synthesis: Some moduli in programming environment Mathematica, Saarbrücken, LAP LAMBERT Academic Publishing (2014), ISBN 978–3–659–53322–8.
- [9] F. Hausdorff, *Set Theory* (2 ed.) (Chelsea Publ., New York, (1962 [1957]) (Republished by AMS–Chelsea 2005), ISBN: 978–0–821–83835–8.
- [10] B. Sendov, *Hausdorff Approximations* (Kluwer, Boston, 1990), doi:10.1007/978-94-009-0673-0
- [11] N. Kyurkchiev, A note on the new geometric representation for the parameters in the fibril elongation process, *Compt. rend. Acad. bulg. Sci.* (2016) (accepted).
- [12] N. Kyurkchiev, On the Approximation of the step function by some cumulative distribution functions, *Compt. rend. Acad. bulg. Sci.* 68(12) (2015) 1475–1482.
- [13] N. Kyurkchiev, S. Markov, On the Hausdorff distance between the Heaviside step function and Verhulst logistic function, *J. Math. Chem.* 54(1) (2016) 109–119, doi:10.1007/S10910-015-0552-0
- [14] N. Kyurkchiev, S. Markov, Sigmoidal functions: some computational and modelling aspects, *Biomath Communications 1*(2) (2014) 30–48, doi:10.11145/j.bmc.2015.03.081
- [15] A. Iliev, N. Kyurkchiev, S. Markov, On the Approximation of the Cut and Step Functions by Logistic and Gompertz Functions, *BIOMATH 4*(2) (2015) 1510101, doi:10.11145/j.biomath.2015.10.101

- [16] A. Iliev, N. Kyurkchiev, S. Markov, On the Approximation of the step function by some sigmoid functions, *Mathematics and Computers in Simulation* (2015), doi:10.1016/j.matcom.2015.11.005
- [17] N. Kyurkchiev, S. Markov, On the approximation of the generalized cut function of degree $p + 1$ by smooth sigmoid functions, *Serdica J. Computing* 9(1) (2015) 101–112.
- [18] N. Kyurkchiev, S. Markov, *Sigmoid functions: Some Approximation and Modelling Aspects*, Saarbrücken, LAP LAMBERT Academic Publishing (2015), ISBN 978–3–659–76045–7.
- [19] V. Kyurkchiev, N. Kyurkchiev, On the Approximation of the Step function by Raised-Cosine and Laplace Cumulative Distribution Functions, *European International Journal of Science and Technology* 4(9) (2016) 75–84.
- [20] N. Kyurkchiev, S. Markov, A. Iliev, A note on the Schnute growth model, *International Journal of Engineering Research and Development* 12 (6) (2016) 47–54.
- [21] N. Kyurkchiev, A. Iliev, On some growth curve modeling: approximation theory and applications, *International Journal of Trends in Research and Development* 3 (3) (2016) 466–471.